

Nitrofurantoin
67-20-9 | DTXSID7020972

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.89e-05 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.41e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylfuran</div> <div>Measured: 1.20e-04</div> <div>Predicted: 66.8</div>	<div>Image not found</div> <div>2,6-Dichlorodiphenyl ether</div> <div>Measured: 3.60e-06</div> <div>Predicted: 9.64e-04</div>	<div>Image not found</div> <div>2,4-Dinitrophenol</div> <div>Measured: 3.90e-04</div> <div>Predicted: 2.01e-04</div>
<div>Image not found</div> <div>Phenyl methyl difluorosilane</div> <div>Measured: 1.22e-04</div> <div>Predicted: 2.86</div>	<div>Image not found</div> <div>2-Nitroaniline</div> <div>Measured: 7.50e-07</div> <div>Predicted: 1.67e-04</div>	